Introduction and Overview of BOUT++ project

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Presented at

2013 BOUT++ Workshop

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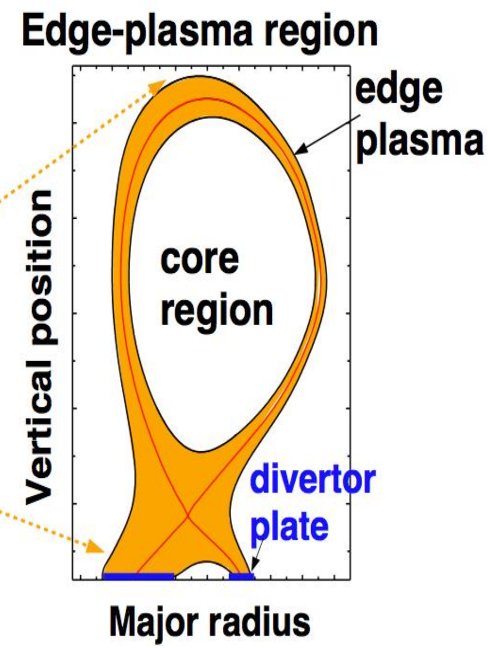
Tokamak edge region encompasses boundary layer between hot core plasma and material walls

- Complex geometry
- Rich physics (plasma, atomic, material)

- Sets key engineering constraints for fusion reactor
- Sets global energy confinement

Tokamak interior



BOUT (BOUndary Turbulence) was originally developed at LLNL in late 1990s for modeling tokamak edge turbulence

BOUT++ is a successor to BOUT, developed in collaboration with Univ. York*

B⭘JT++
Boundary Plasma Turbulence Code

Original BOUT, tokamak applications on boundary turbulence and ELMs with encouraging results

BOUT-06: code refactoring using differential operator approach, high order FD, verification

BOUT++: OOP, 2D parallelization, applications to tokamak ELMs and linear plasmas

- ✓**Gyro-fluid extension**
- ✓**RMPs**
- ✓**Neutrals & impurities**
- ✓**Preconditioner**
- ✓**Computing on GPUs**

2000 2005 2013

- ***X.Q. Xu and R.H. Cohen, Contrib. Plasma Phys. 38, 158 (1998)***
- ***Xu, Umansky, Dudson & Snyder, CiCP, V. 4, 949-979 (2008).***
- **Umansky, Xu, Dudson, et al., , Comp. Phys. Comm. V. *180 , 887-903 (2008).***
- **Dudson, Umansky, Xu et al., Comp. Phys. Comm. V.180 (2009) 1467.**
- **Xu, Dudson, Snyder et al., PRL 105, 175005 (2010).**

BOUT and BOUT++ have been products of broad international collaborations

The University of York

The University of California UCLA

General Atomics

Argonne National Laboratory

Illinois Institute of Technology

CCFE Culham Centre for Fusion Energy

IFS Theory Group Institute for Fusion Studies

UCSD

Berkeley Lab

Lawrence Berkeley National Laboratory

Lawrence Livermore National Laboratory

JAEA

Lodestar Research Corporation

MIT PSFC

NFRI 국가핵융합연구소 National Fusion Research Institute

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SWIP

Southwestern Institute of Physics

Institute of plasma Physics Chinese Academy of Sciences

The University of Wisconsin Madison

ifts 浙江大學聚變理論與模擬中心

Institute for Fusion Theory and Simulation, Zhejiang University

University of Science and Technology of China 1958

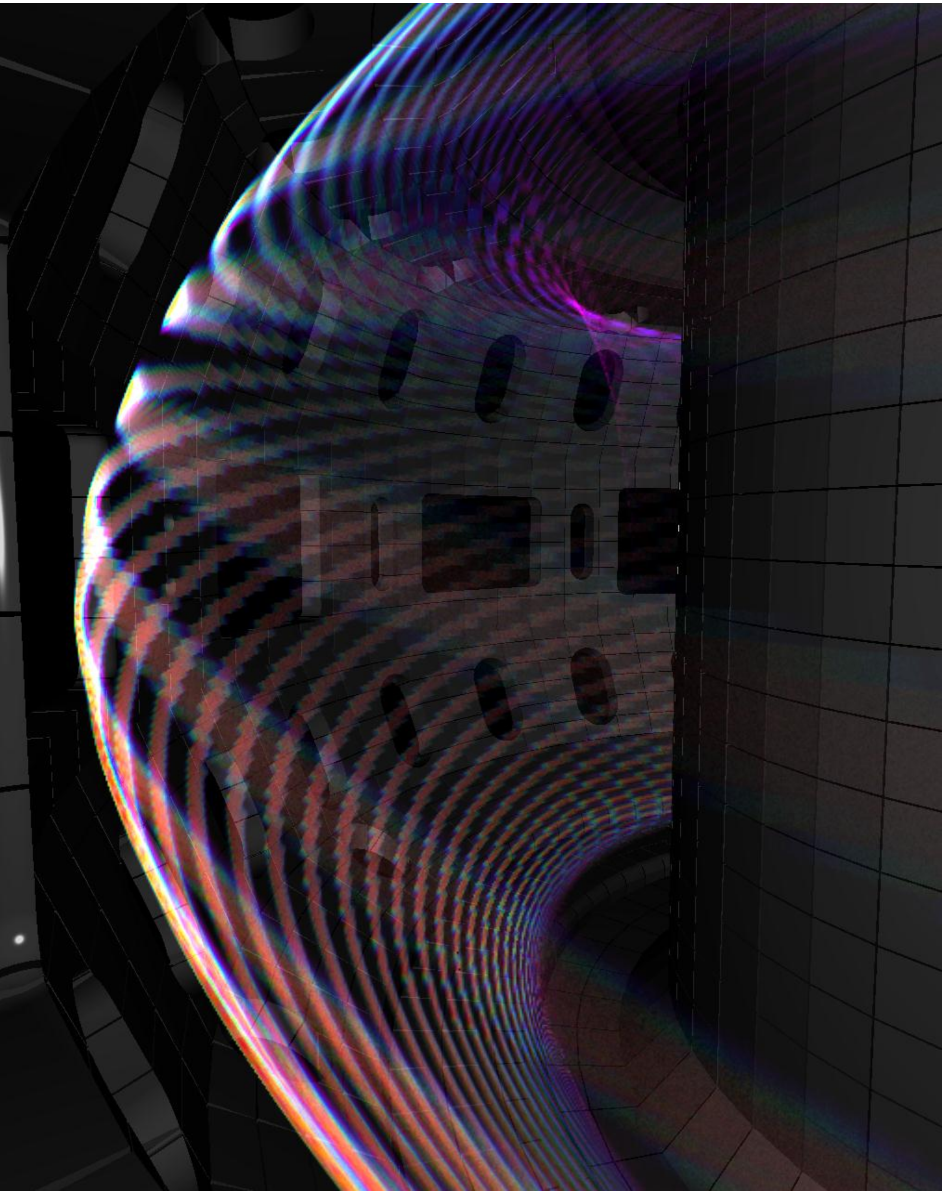
北大聚变模拟中心

Fusion Simulation Center, Peking University

BOUT++ MAP


Arctic Ocean
Arctic Ocean
Greenland
Iceland
Finland
Sweden
Norway
Russia
Canada
Poland
Germany
Ukraine
Kazakhstan
Mongolia
France
Italy
Spain
Turkey
United States
Japan
North Atlantic Ocean
Iraq
Iran
Afghanistan
Pakistan
Algeria
Libya
Egypt
Saudi Arabia
India
Mexico
Thailand
Mali
Niger
Sudan
Chad
Nigeria
Ethiopia
Venezuela
Colombia
Kenya
DR Congo
Indonesia
Papua New Guinea
Tanzania
Brazil
Peru
Angola
Bolivia
Namibia
Botswana
Madagascar
Indian Ocean
South Pacific Ocean
Chile
South Atlantic Ocean
Australia
South Africa
Argentina
New Zealand

Principal Results since 2011 BOUT++ workshop



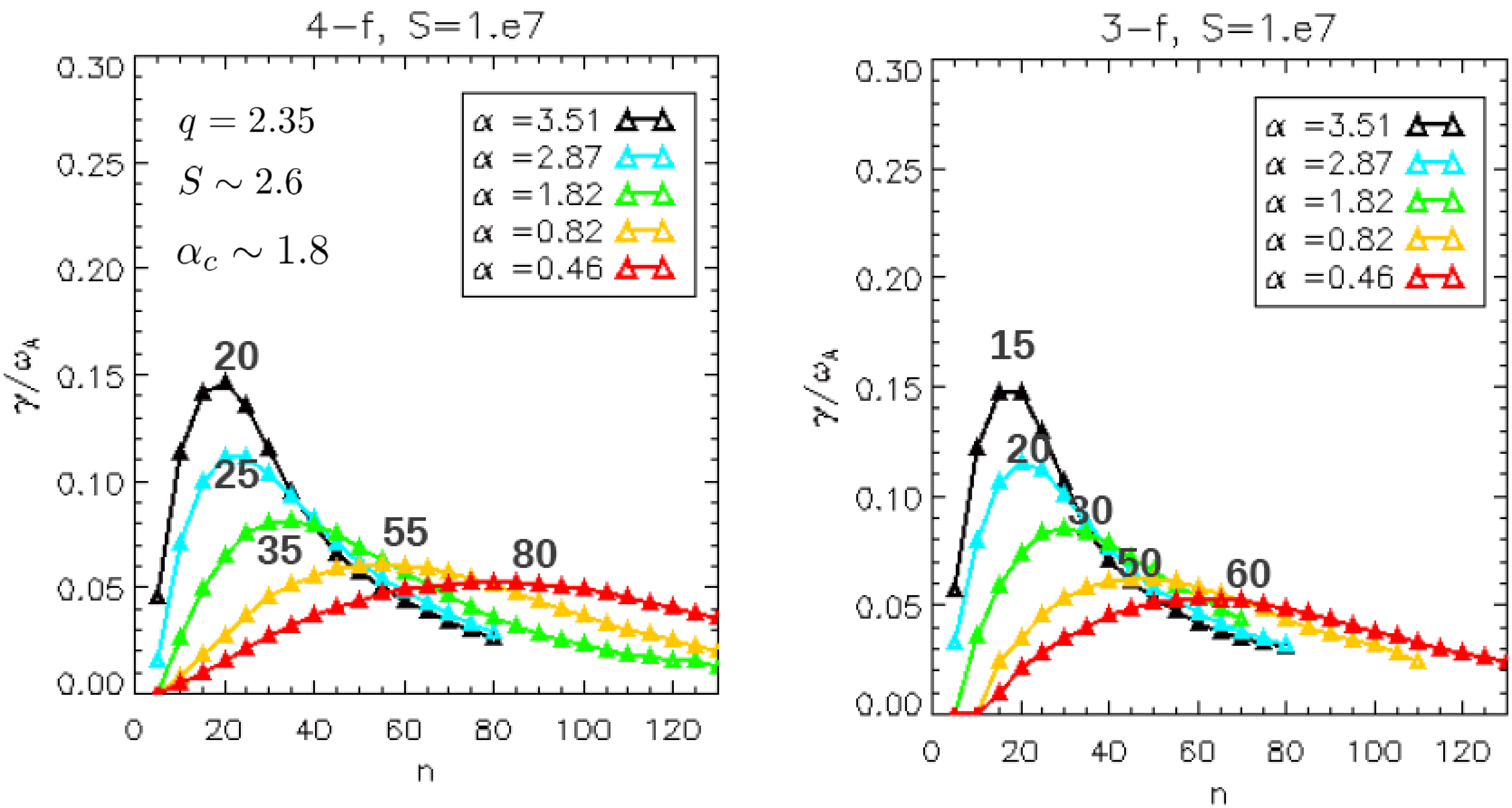
- A suite of two-fluid models has been implemented in BOUT++ for
  - ✓ different ELM regimes and fluid turbulence
- A suite of gyro-fluid models is under development for
  - ✓ pedestal turbulence and transport
- Neutral models
  - ✓ Fluid neutral models are developed for
    - SMBI, GAS puffing, Recycling
  - ✓ Coupled to EIRENE Monte Carlo code to follow the neutral particles.
- Developed Physics-based preconditioning based on Chacon's presentation at 2011 BOUT++ workshop
- We find that nonlinear mode coupling can shift the linear P-B mode stability threshold, which may explain those puzzles observed in ELM experiments.

BOUT++: A framework for nonlinear twofluid and gyrofluid simulations ELMs and turbulence

- **Different twofluid and gyrofluid models are developed under BOUT++ framework for ELM and turbulence simulations**

Twofluid	Gyrofluid	Physics
3-field $(\varpi, P, A_\parallel)$	**1+0** $(n_{iG}, n_e, A_\parallel)$	**Peeling-ballooning mode**
4-field $(\varpi, P, A_\parallel, V_\parallel)$	**2+0** $(n_{iG}, n_e, A_\parallel, V_\parallel)$	**+ acoustic wave**
5-field $(\varpi, n_i, A_\parallel, T_i, T_e)$		**+ Thermal transport no acoustic wave**
6-field $(\varpi, n_i, A_\parallel, V_\parallel, T_i, T_e)$ **Braginskii equations**	**3+1** $(n_{iG}, n_e, A_\parallel, V_\parallel, T_{i\perp}, T_{i\parallel}, T_e)$ Snyder+Hammett's model	**+ additional drift wave instabilities + Thermal transport**

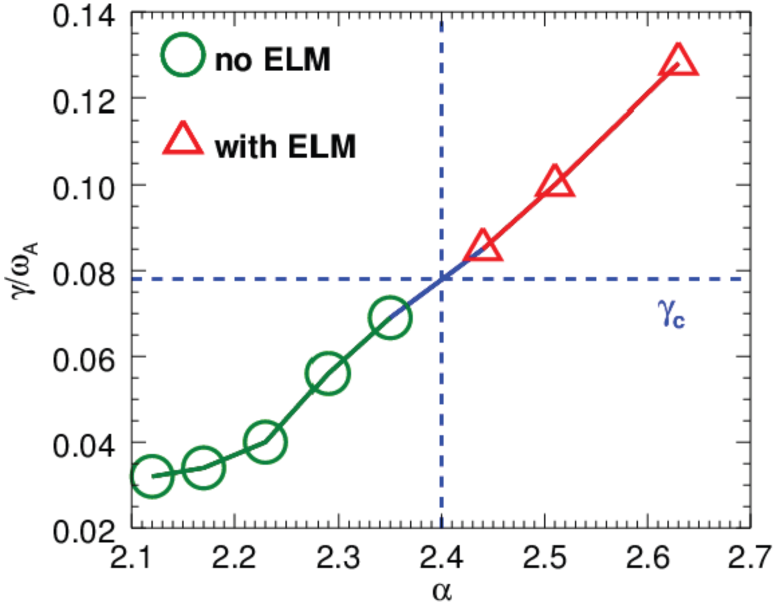
4-field model agrees well with 3-field for both ideal and resistive ballooning modes

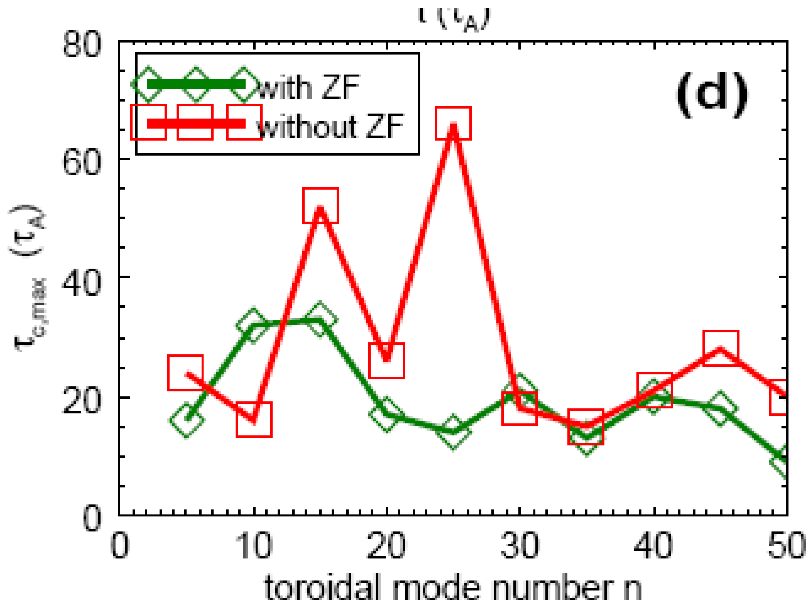


- α_c value from eigenvalue solver agrees with BOUT simulation.
- Non-ideal effects are consistent in both models
  - ✓ diamagnetic stabilization
  - ✓ resistive mode with $\alpha < \alpha_c$
  - ✓ increase n of maximum growth rate with decrease of α

T. Rhee, et al.

The onset of ELMs $\gamma > 0$ is shifted to $\gamma > \gamma_c$ due to P-B turbulence, which may explain those unknown questions observed in experiments





- ✓ **The occurrence of ELMs depends sensitively on the nonlinear dynamics of P-B turbulence;**
- ✓ **The evolution of relative phase between P-B mode potential and the pressure perturbations is a key to ELMs**
- ✓ **Phase coherence time τ_c determines the growing time of an instability by extraction of expansion free energy.**
- ✓ **Nonlinear criterion sets the onset of ELMs**

$$\gamma_c \sim \ln 10 / \tau_c$$

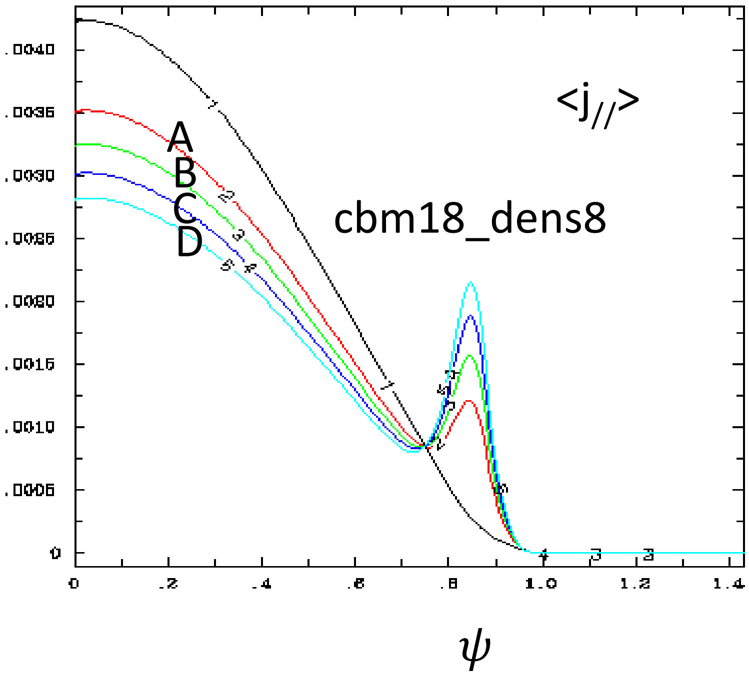
$$\delta\varphi(n,\psi,\theta,t) = \arg\left(\frac{\hat{P}_n(\psi,\theta,t)}{\hat{\phi}_n(\psi,\theta,t)}\right)$$

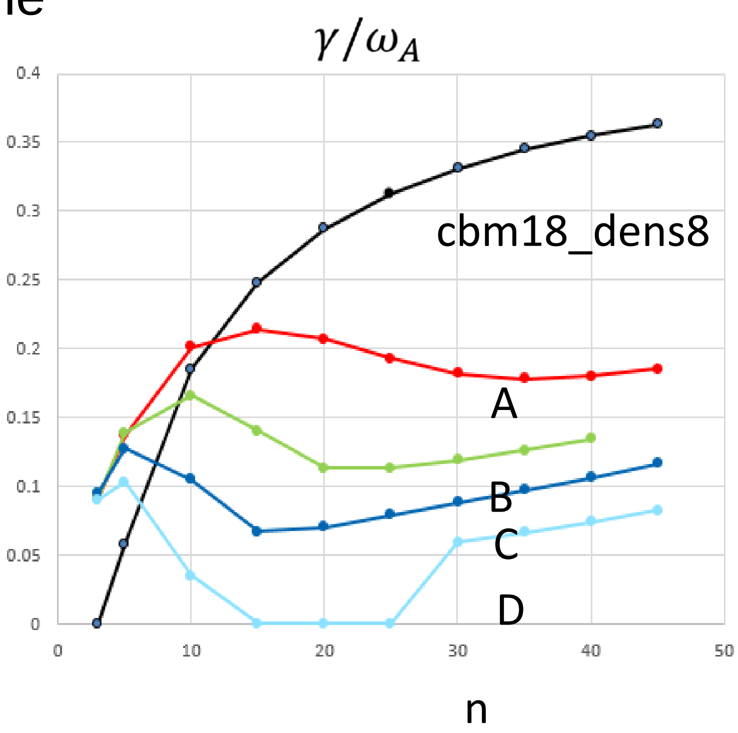
P. W. Xi, X.Q. Xu, P. H. Diamond, submitted to PRL, 2013

Linear calculations of edge current driven modes

(G Q Li, et al.)

- With CORSICA, a sequence of equilibria with different edge current was created and the total current was fixed
- As the edge current increased, the high n ballooning modes were stabilized, the dominant mode changed from ballooning modes to low n kink mode
- The ballooning stabilization effect is due to the local shear increasing at the outer mid-plane





BOUT++ global GLF model agrees well with gyrokinetic results

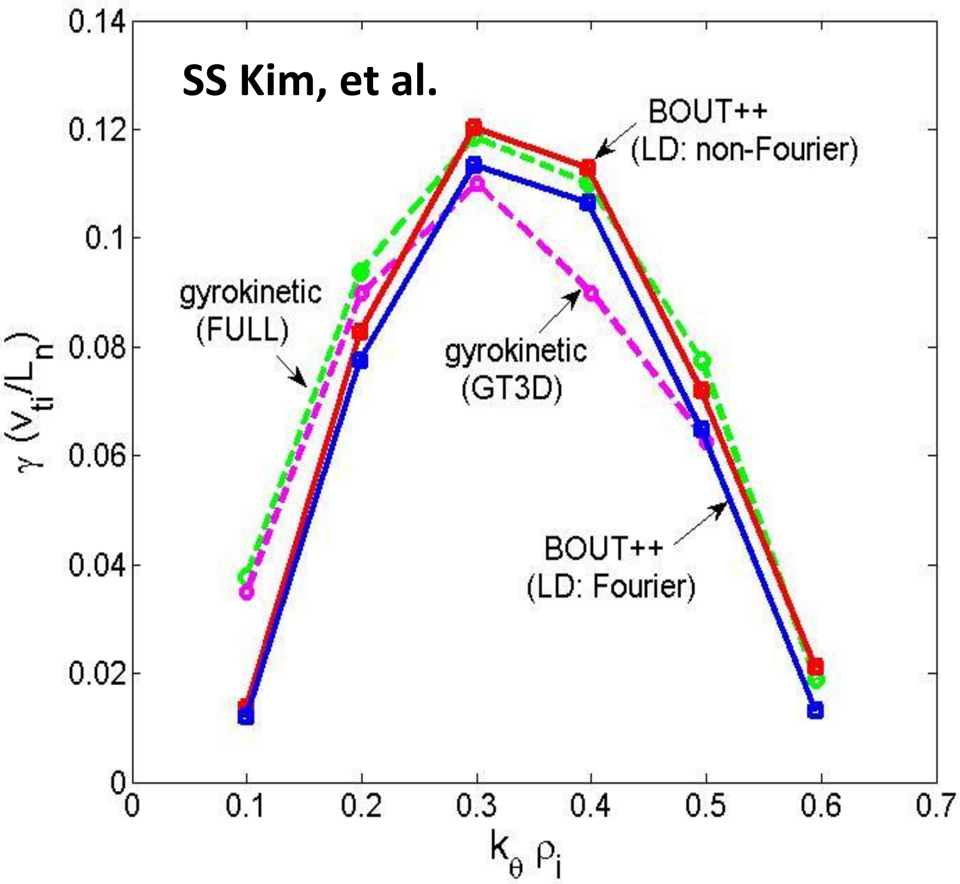
- **BOUT++ using Beer's 3+1 model agrees well with gyrokinetic results.**
- **Non-Fourier method for Landau damping shows good agreement with Fourier method.**

✓ **Implemented in the BOUT++**
  - ✓ **Padé approximation for the modified Bessel functions**
  - ✓ **Landau damping**
  - ✓ **Toroidal resonance**
  - ✓ **Zonal flow closure in progress**
  - ✓ **Nonlinear benchmark underway**

✓ **Developing the GLF models**
  - ✓ to behave well at large perturbations
  - ✓ for second-order-accurate closures

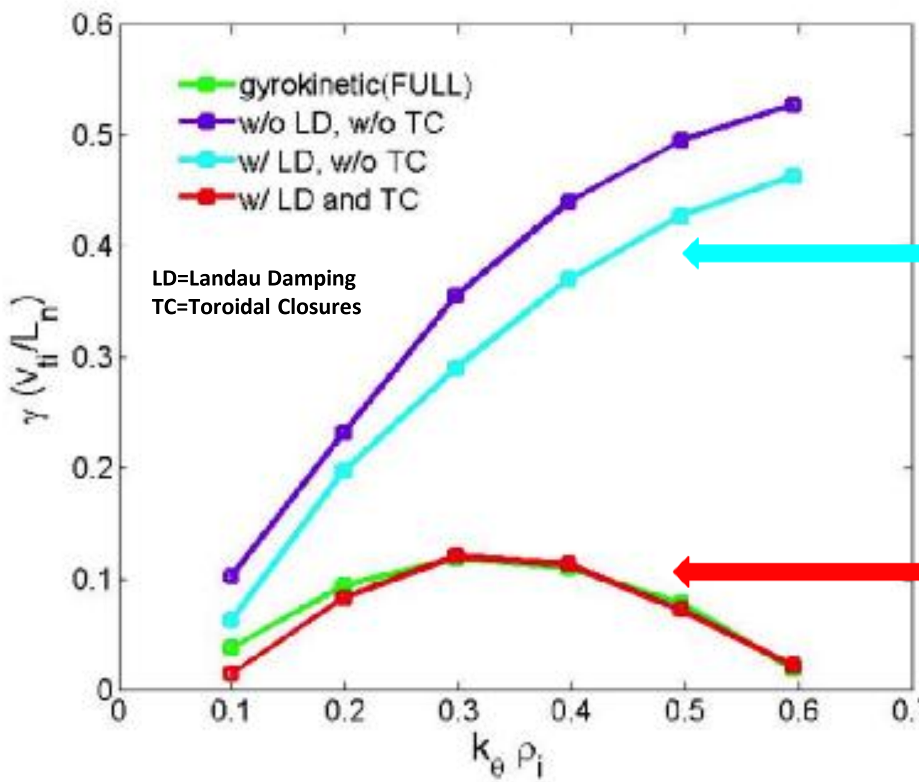
✓ **Conducting global nonlinear kinetic ITG/KBM simulations at pedestal and collisional drift ballooning mode across the separatrix in the SOL**

Cyclone base case



Our GLF implementation gives excellent agreement with gyrokinetic calculations for ITG instability growth rates

- The accuracy of the fluid moment approach improves as the set of closure terms becomes more complete



FY12 accomplishment

FY13 accomplishment

The Landau-fluid closure terms are essential for achieving agreement with gyrokinetic calculations

A. Dimits, SS Kim, et al.

Extension of Gyro-Landau fluid (GLF) closures (Joseph, et al)

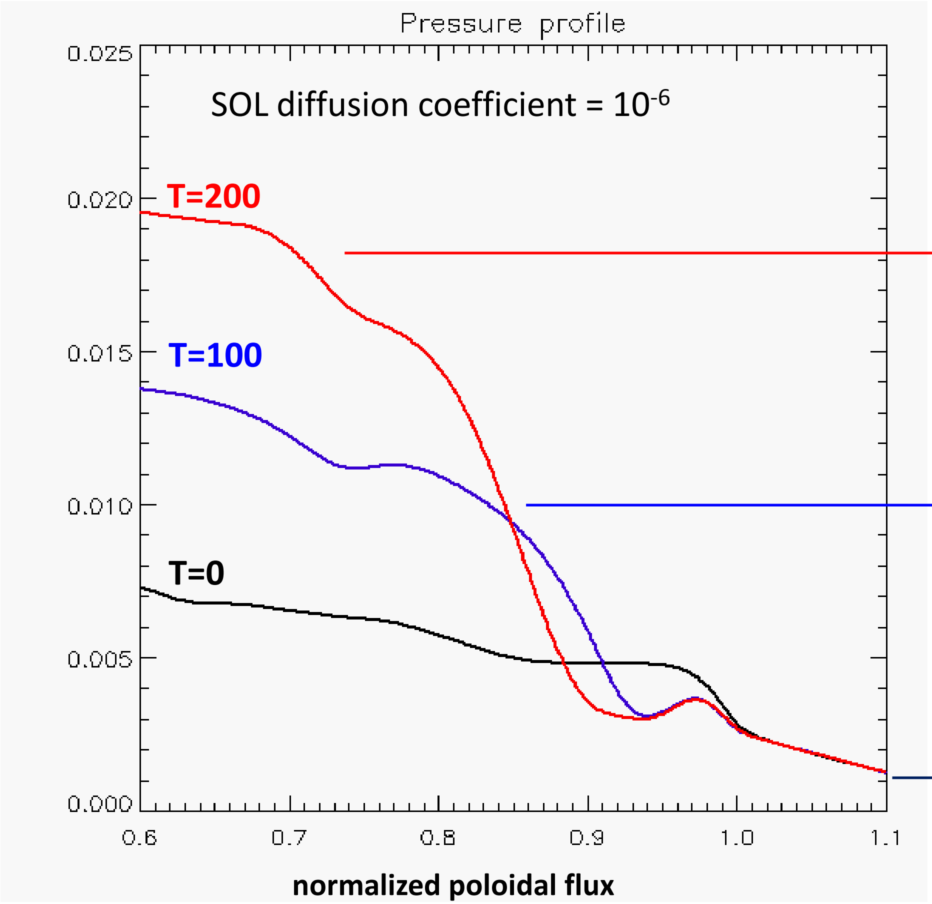
- **Previous GLF equations yield high accuracy to 1st order in δ**
  - ✓ Yields accurate linear growth rates & eigenfunctions

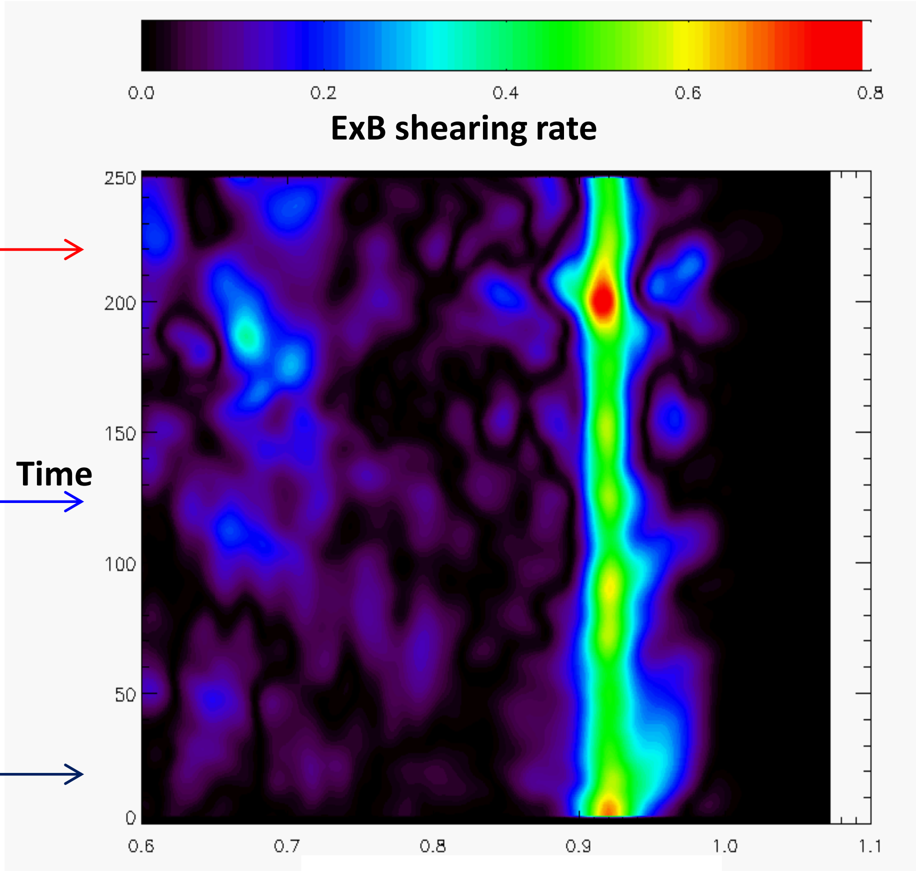
- **In previous approaches, not all nonlinearities were retained and are rarely implemented**
  - ✓ Fluid moments naturally generate a number of nonlinear terms (particularly $V_{||}$)
  - ✓ Typically, nonlinear <ExB> drifts and parallel <E·B*> forces are only retained approximately through perpendicular and parallel "nonlinear phase mixing closures" (Dorland & Hammett POP 1992)

- **Our goal is to develop GLF equations consistently to 2nd order in**
  - ✓ Hamiltonian approach to perpendicular closures ensures conservation of energy and momentum
  - ✓ Implies that nonlinear polarization is closely related to nonlinear <ExB> drifts
  - ✓ "Chang-Callen" (POP 1992) approach to parallel closures generates a systematic method for accurate inclusion of Coulomb collisions
  - ✓ We are developing neoclassical closures for axisymmetric modes & zonal flows

Development of flux-driven edge simulation
Edge Transport Barrier formation with external sheared flow

- Heat source inside the separatrix and sink outside the separatrix
- ETB is formed by the externally applied sheared flow, but sometimes triggered by turbulence driven flow when external flow is zero

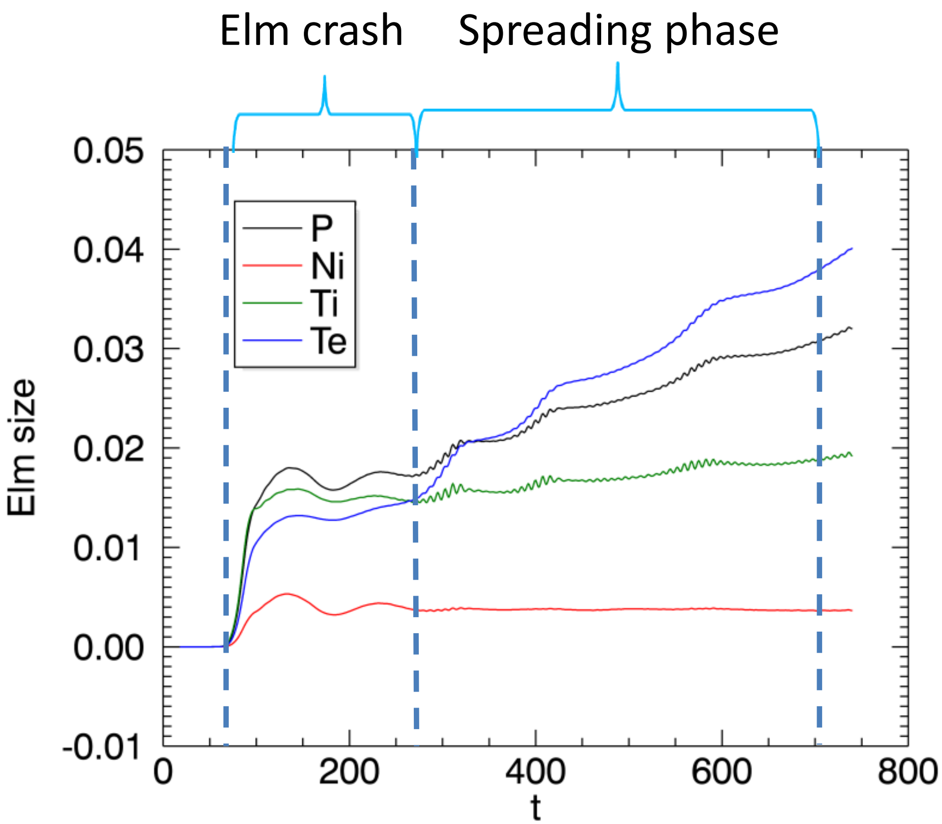




G Y Park, et al., POSTER SESSION II

6-field simulations show the separation of particle and energy transport channels

- ELM has fast crash phase and slow perturbation spreading phase
- Ion perturbation has larger initial crash
- Electron provides large turbulence spreading
- The difference of ion and electron dynamics is resulting from parallel physics due to the mass ratio.



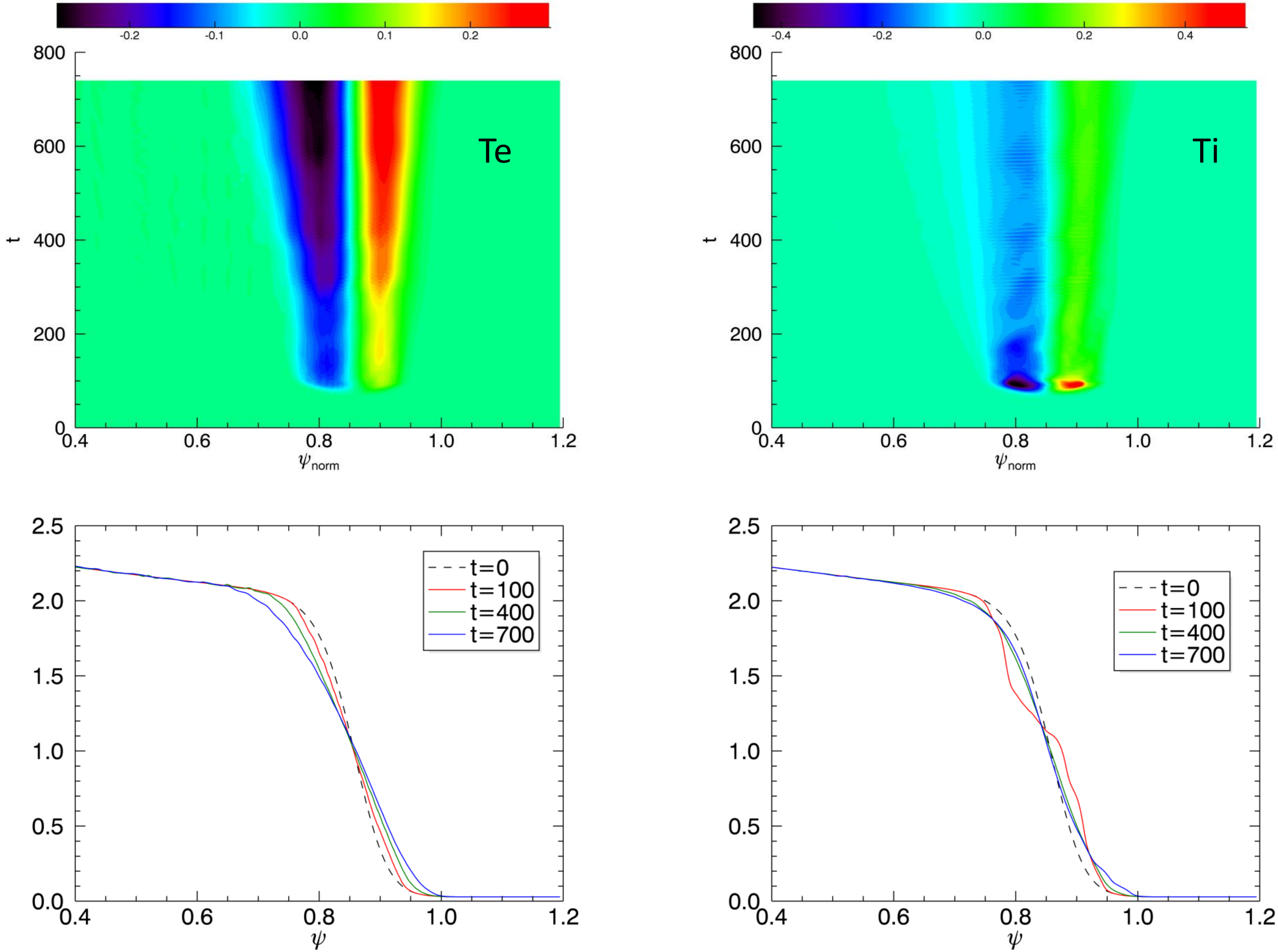
* Definition of ELM size:

$$\Delta_{ELM}^{th} = \frac{\Delta W_{ped}}{W_{ped}} = \frac{\langle \int_{R_{in}}^{R_{out}} \oint dR d\theta (P_0 - \langle P \rangle_\zeta) \rangle_t}{\int_{R_{in}}^{R_{out}} \oint dR d\theta P_0},$$

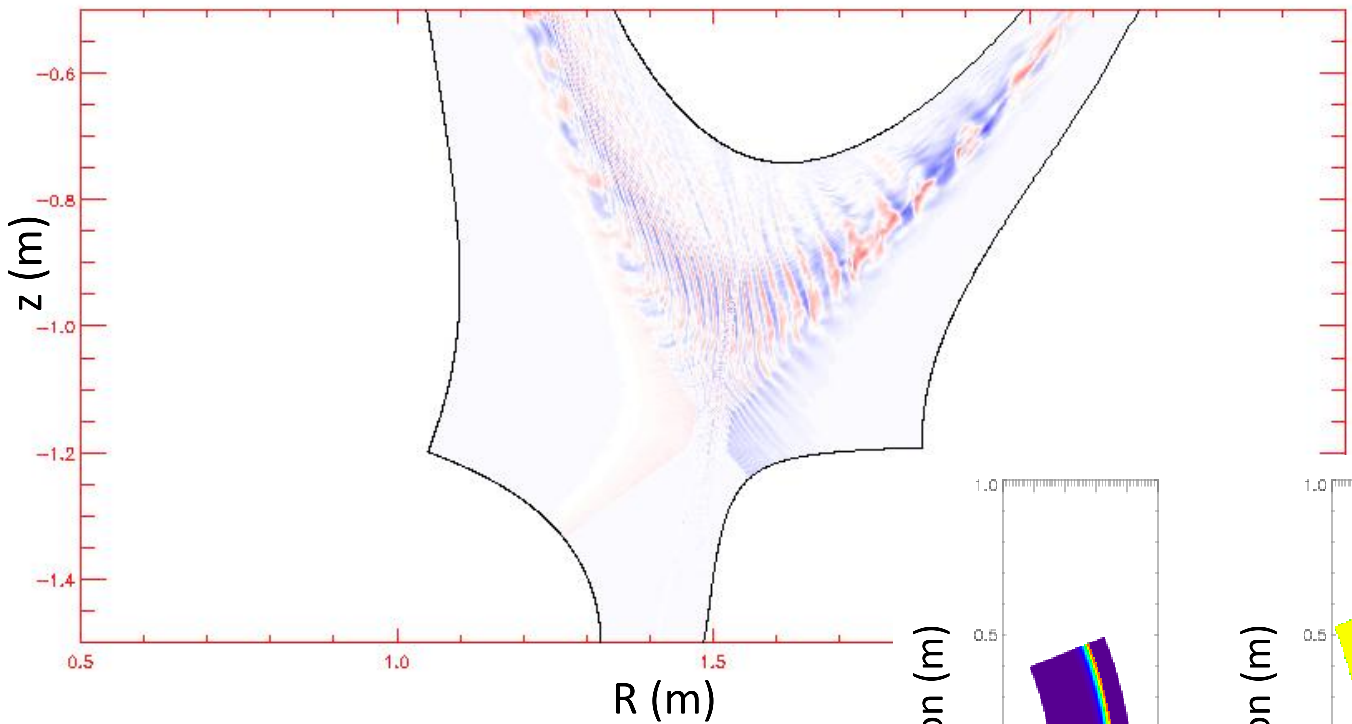
C. H. Ma, et al., POSTER SESSION II

Ion perturbation has a large initial crash and electron perturbation only has turbulence spreading due to inward ExB convection

(C. H. Ma, et al., POSTER SESSION II)

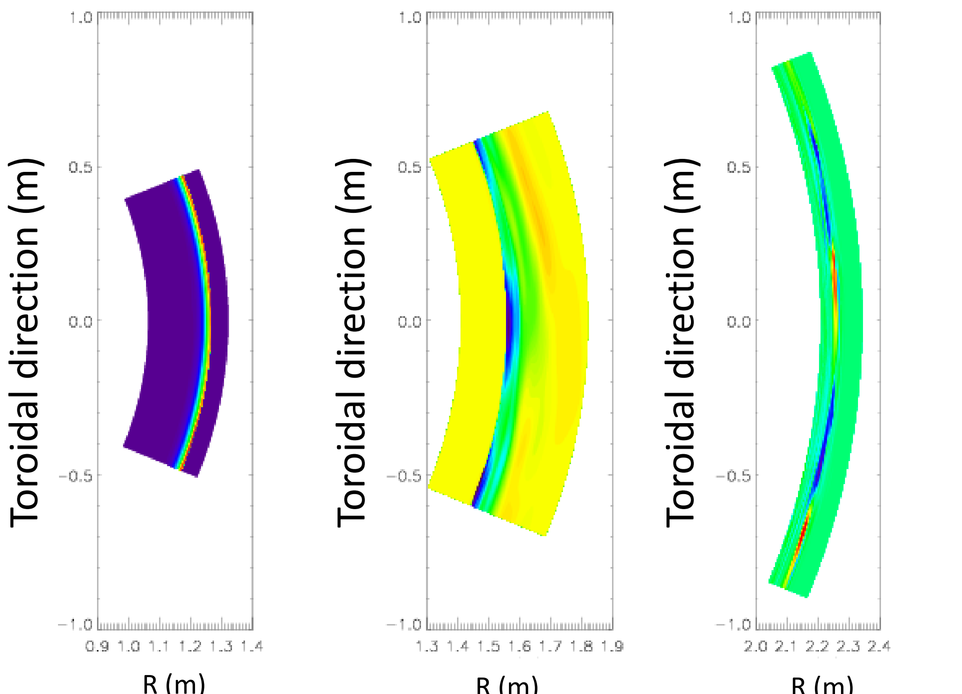


6-field module has the capability to simulate the heat flux in divertor geometry



Left: heat flux distribution around x-point

Bottom: heat flux structures on toroidal direction.



Inner target Outer target Outer mid-plane

Six-field (ϖ, n_i, T_i, T_e, $A_{||}$, $V_{||}$): based on Braginskii equations, the density, momentum and energy of ions and electrons are described in drift ordering [1,2].

[1]X. Q. Xu et al., Commun. Comput. Phys. **4**, 949 (2008).
[2]T. Y. Xia et al., *Nucl. Fusion* **53**, 073009 (2013).

Neutral fluid model has been implemented in BOUT++
Processes of Molecule Reaction

Franck-Condon

- ✓ **SMBI**
- ✓ **GAS puffing**
- ✓ **recycling**

Molecules → Atoms → Ionization → Plasmas

$$H_2 \Rightarrow 2H^0 \Rightarrow 2H^+ + 2e$$

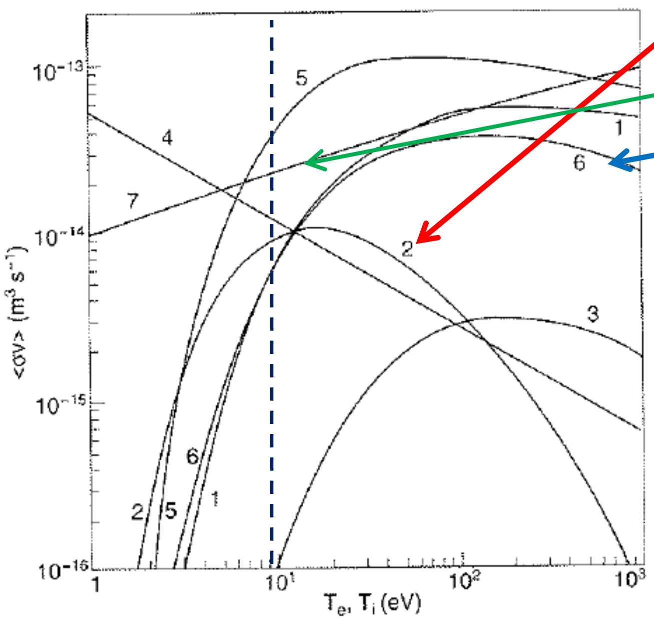
Dissociation

$$e + H_2 \rightarrow 2H^0 + e$$

Charge Exchange(CX)

$$H^+ + H^0 \rightarrow H^0 + H^+$$

$$e + H^0 \rightarrow H^+ + 2e$$



At Edge plasma

$$\boxed{\left\langle \sigma V \right\rangle_{diss}} \approx \boxed{\left\langle \sigma V \right\rangle_{I}} < \boxed{\left\langle \sigma V \right\rangle_{CX}}$$

$$\left\langle \hat{\sigma}_I \hat{V}_{th,e} \right\rangle \approx \left\langle \hat{\sigma}_{diss} \hat{V}_{th,e} \right\rangle = 3\times10^{-8} \left(0.1T_e eV\right)^2 / \left[3 + \left(0.1T_e eV\right)^2\right] cm^3/s$$

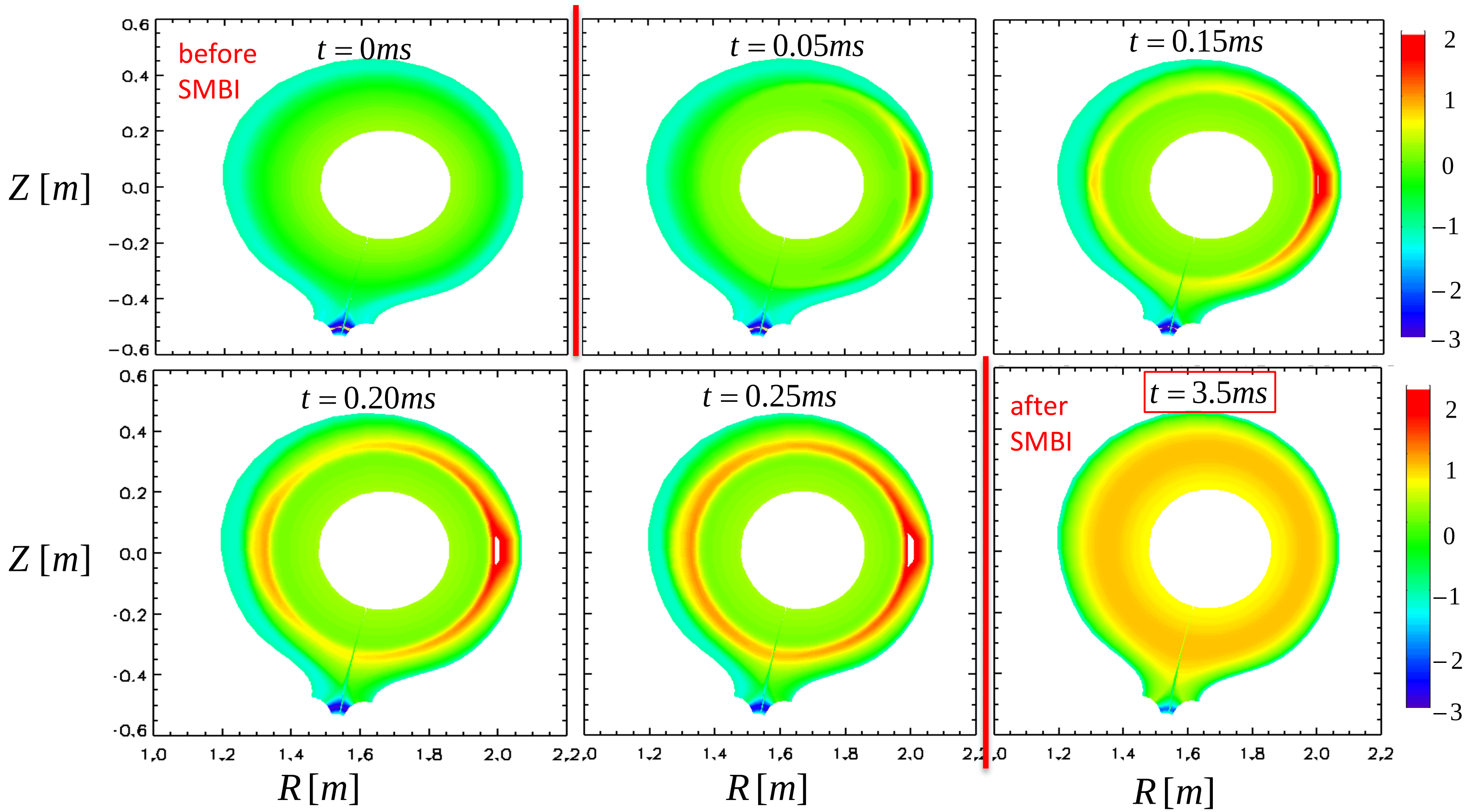
$$\left\langle \sigma_{CX} V_{th,i} \right\rangle = 1.7\times10^{-8} + 1.9\times10^{-8} \frac{\left(1.5T_i eV\right)^{1/3} - \left(15eV\right)^{1/3}}{\left(150T_i eV\right)^{1/3} - \left(15eV\right)^{1/3}} cm^3/s$$

Figure 1.25. The rate coefficients for atomic and molecular hydrogen [1.23]. The numbered reactions are (1): $e + H_2 \rightarrow H_2^+ + 2e$, (2): $e + H_2 \rightarrow 2H^0 + e$, (3): $e + H_2 \rightarrow H^0 + H^+ + 2e$, (4): $e + H_2^+ \rightarrow 2H^0$, (5): $e + H_2^+ \rightarrow H^0 + H^+ + e$, (6): $e + H^0 \rightarrow H^+ + 2e$, and charge exchange (7): $H^0 + H^+ \rightarrow H^+ + H^0$.

Peter C. Stangeby *The Plasma Boundary of Magnetic Fusion Devices*, Institute of Physics publishing, 2000

Poloidal Propagation of Plasma Density Blobs During SMBI due to Poloidal Convection Effects

$$\log(N_i[N_0]) \qquad N_0 = 1\times 10^{19}/m^3$$

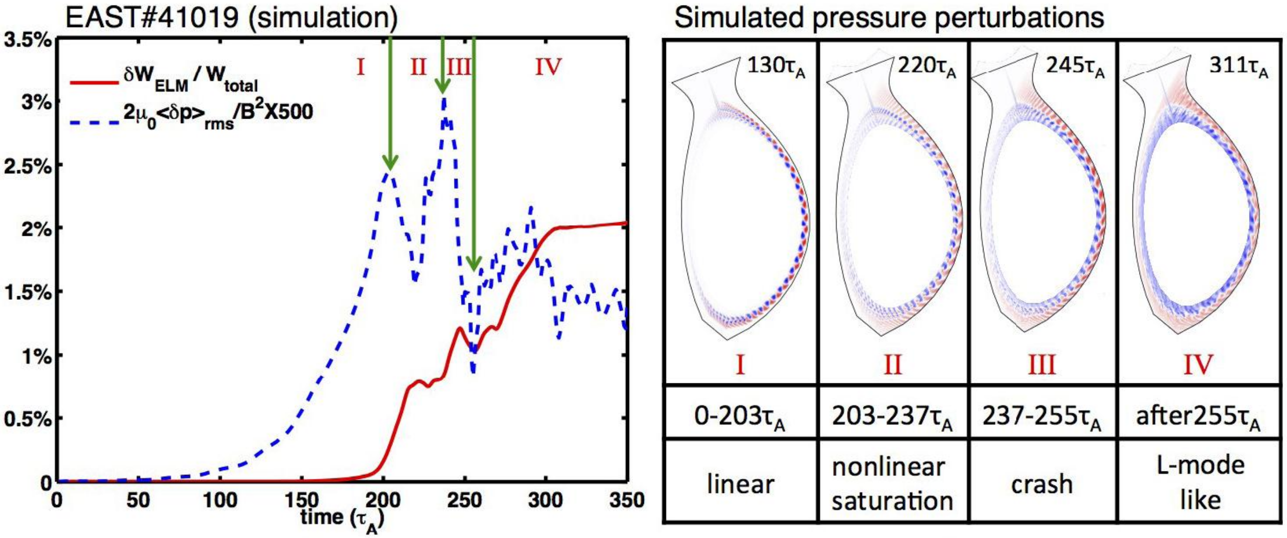


SMBI creates poloidal density blobs locally which then are propagating poloidally

Z. H. Wang, X.Q.Xu, T. Y. Xia, and T. D. Rognlien, submitted to Nuclear Fusion, 2013

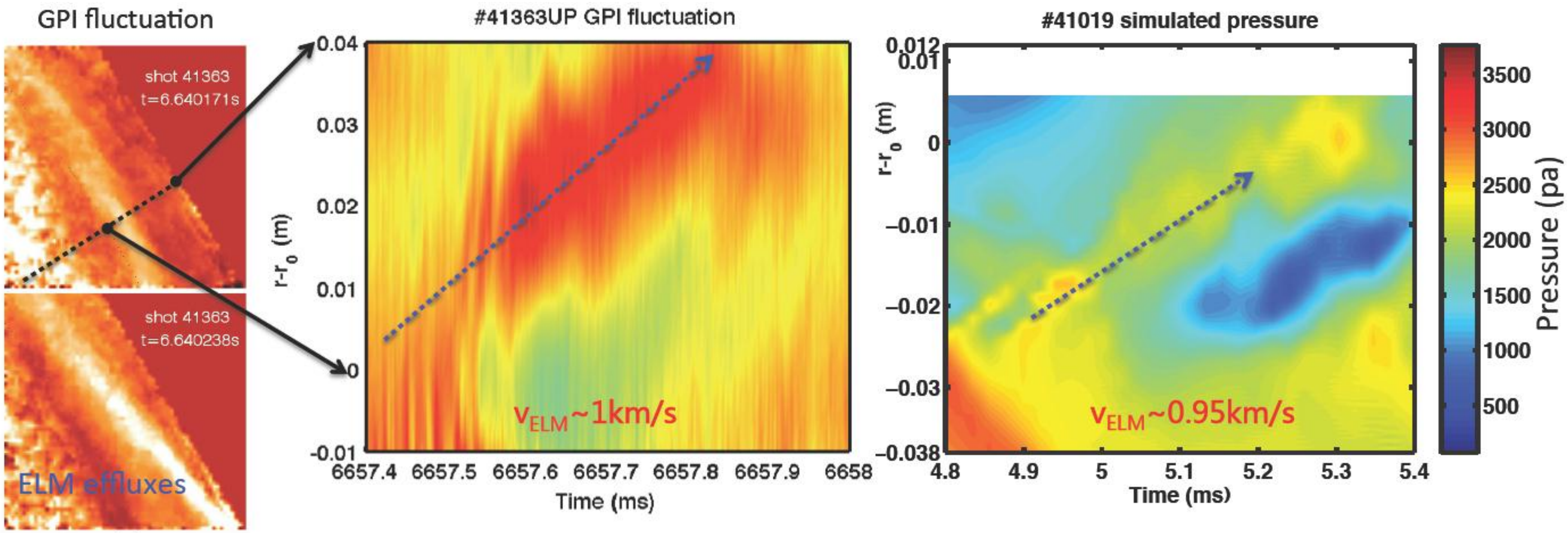
Ongoing validation of MHD instability data from EAST

3D nonlinear simulations of ELM with X-point geometry



(a) (b)

Z. X. Liu, X. Q. Xu, et al, "3D nonlinear simulation of ELM with X-point geometry on the EAST Tokamak", submitted to PRL (2013).



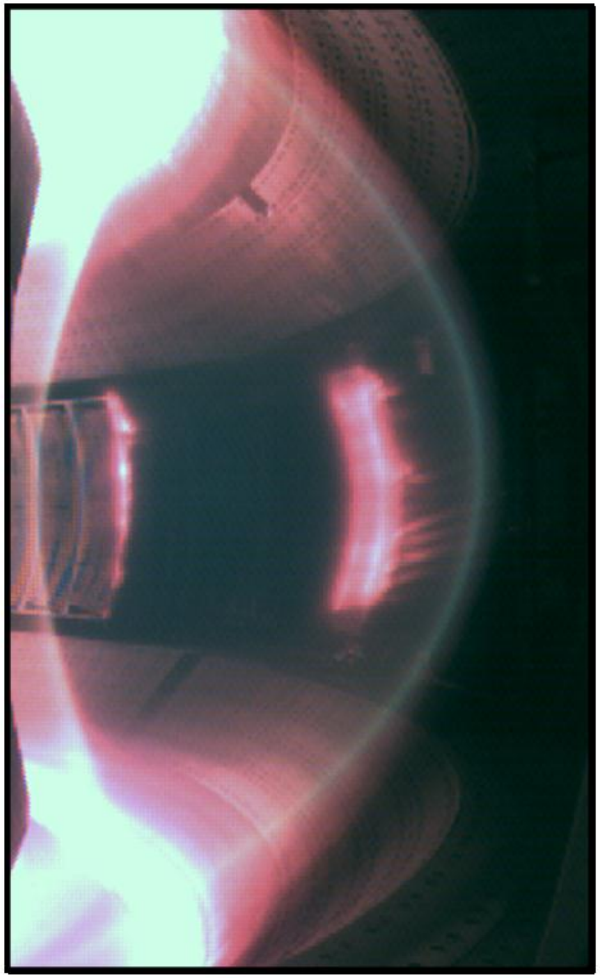
(a) (b) (c)

Ongoing validation of MHD instability data from EAST

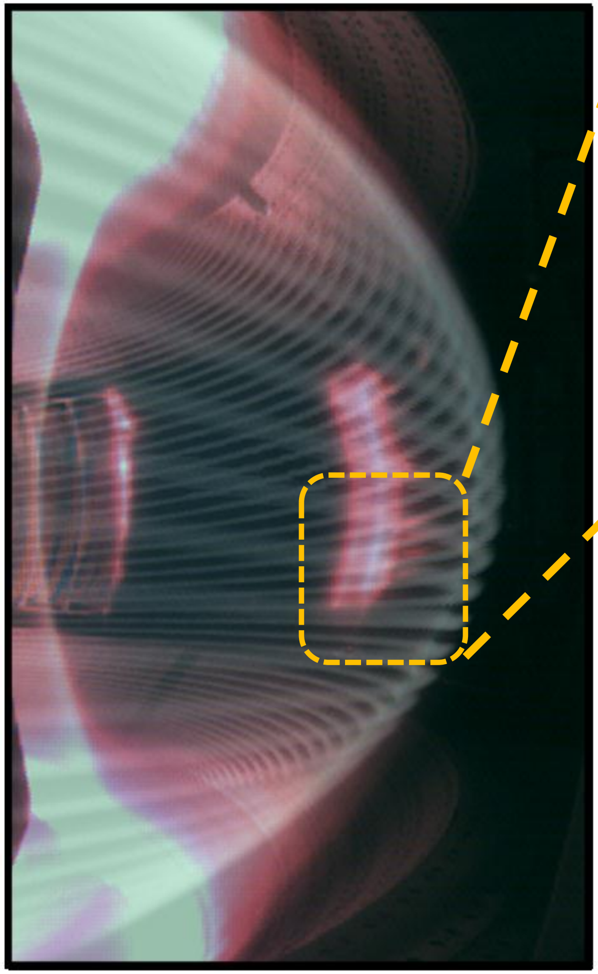
BOUT++ simulations show that the stripes from EAST visible camera match ELM filamentary structures

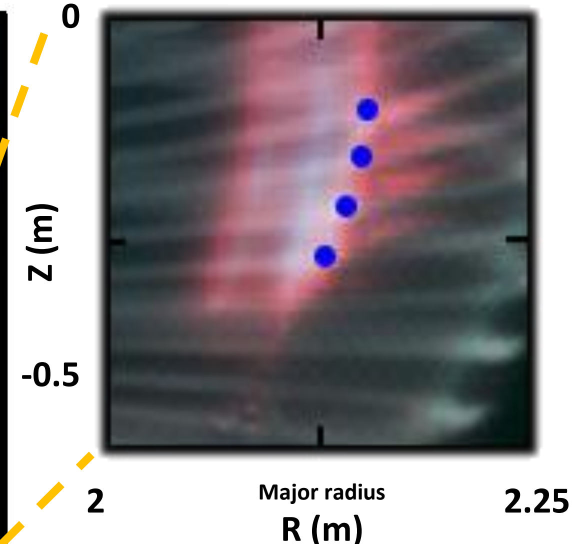
Z.X.Liu, et al., POSTER SESSION I

EAST#41019@3034ms Visible camera shows bright ELM structure$



BOUT++ simulation shows that the ELM stripe are filamentary structures*





- Pitch angle match!
- Mode number match!

T. Y. Xia, X.Q. Xu, Z. X. Liu, et al, TH/5-2Ra, 24th IEAE FEC, San Diego, CA, USA, 2012

$Photo by J. H. Yang
*Figure by W.H. Meyer

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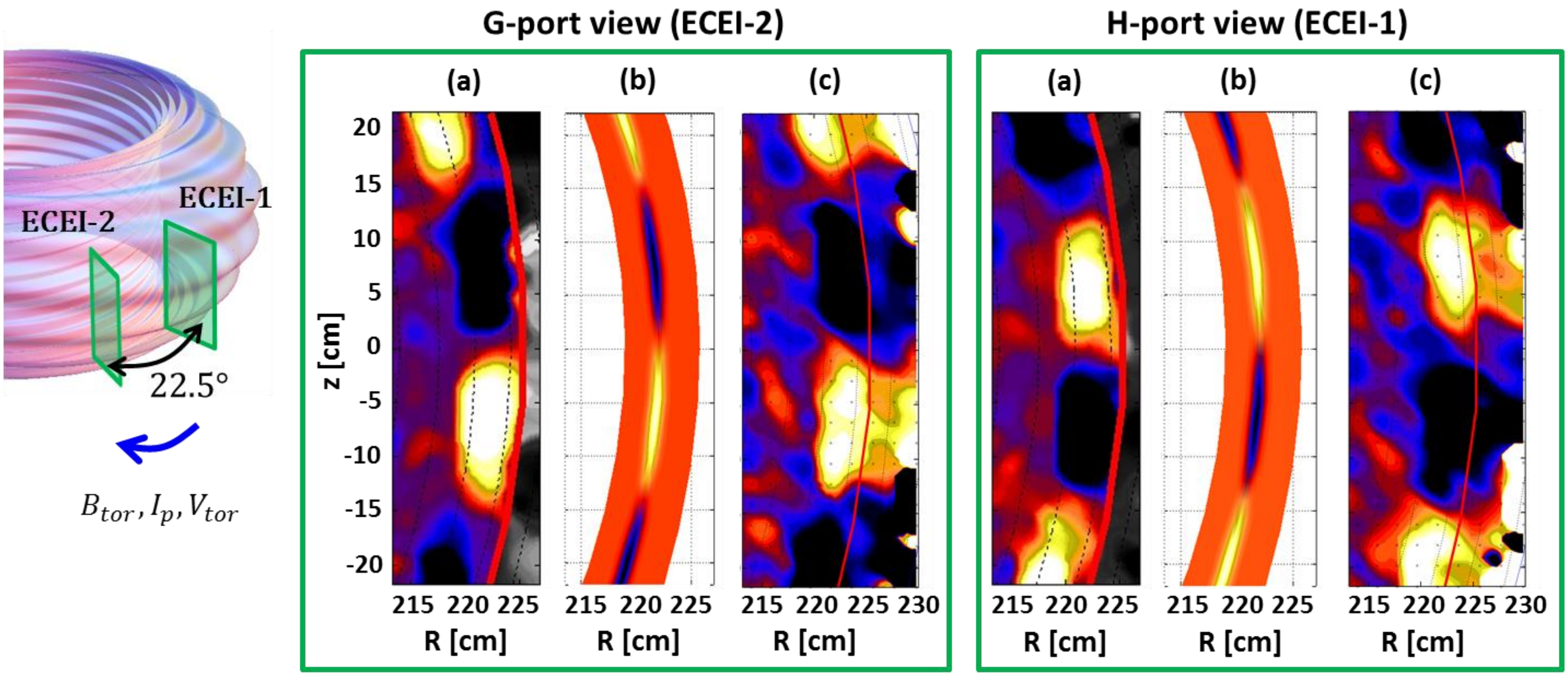
Ongoing validation of MHD instability data from KSTAR

The synthetic images from interpretive BOUT++ simulations show the similar patterns as ECEI

H Park, et al., APS DPP invited talk, Nov., 2013



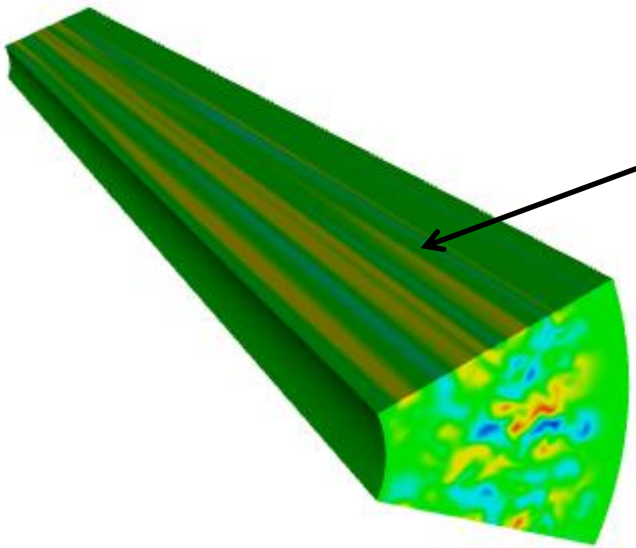
(a) ECE-images at KSTAR discharge #7328, t ~ 4.36 (s)

(b) n = 8 BOUT++ linear simulations

(c) Synthetic images from the simulations with system noise

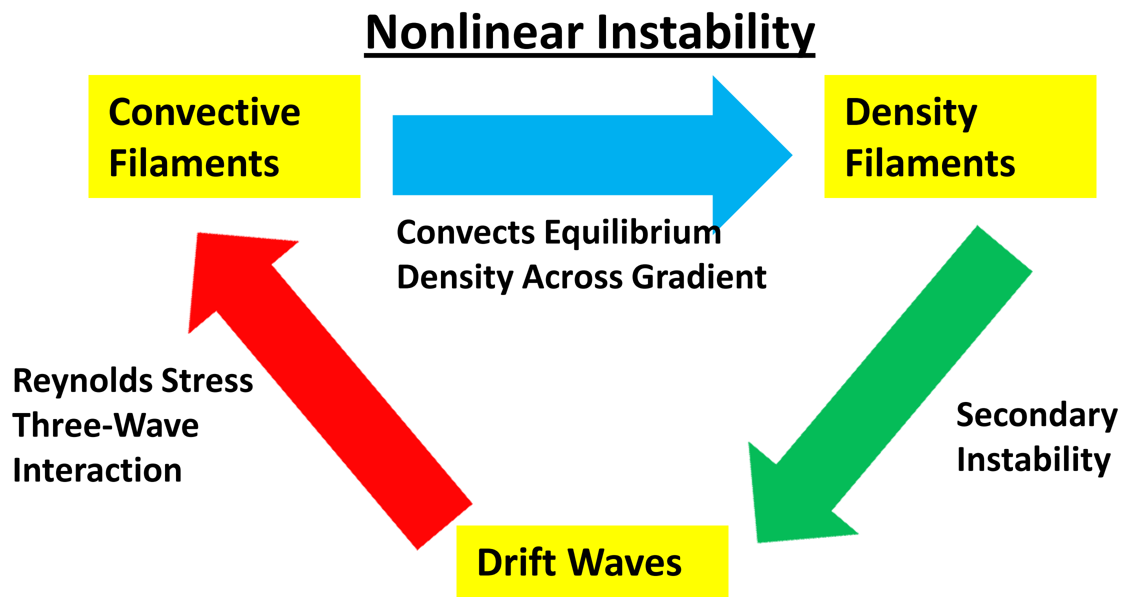
M. Kim, et al., POSTER SESSION I

Nonlinear instability found in simulations of Large Plasma Device (LAPD) turbulence



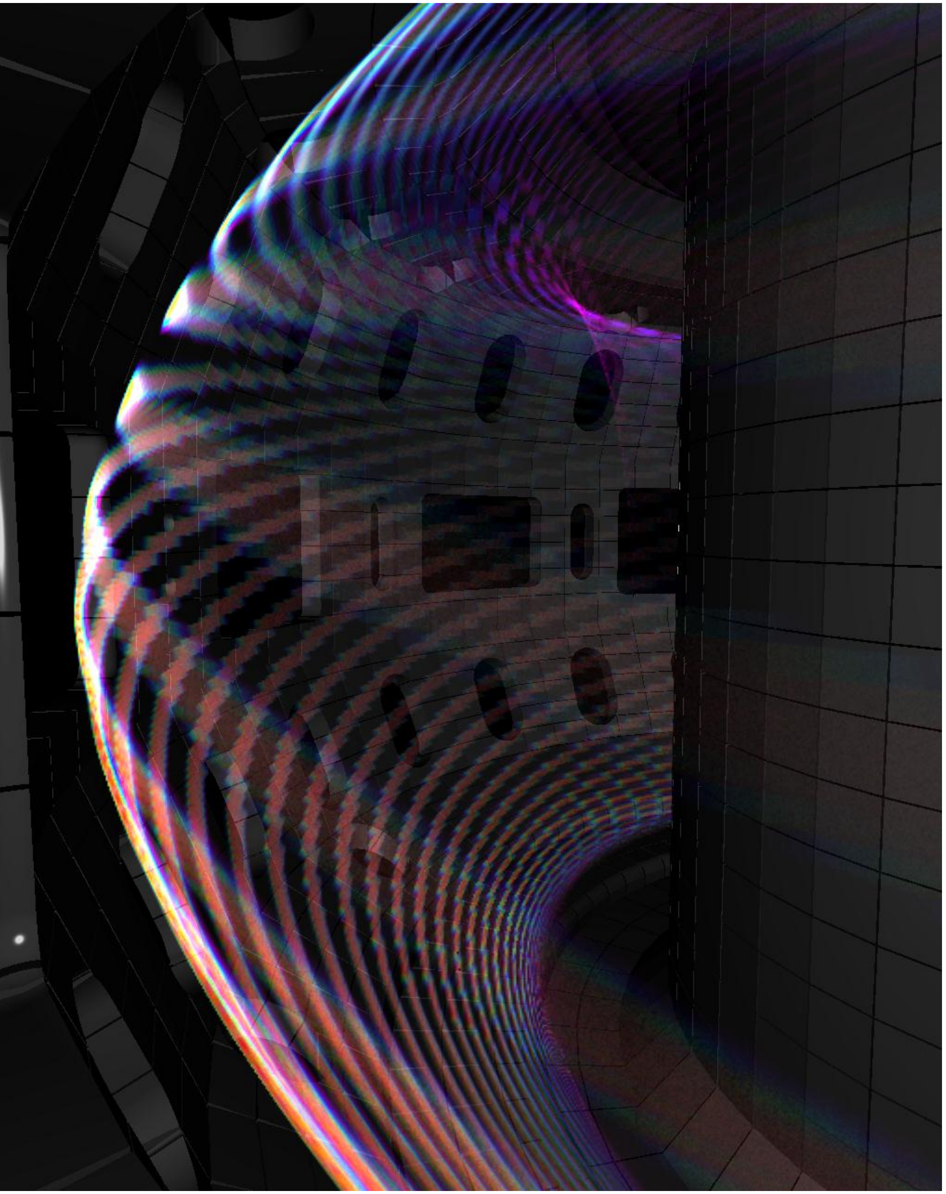
Filamentary Structures Spanning Entire Machine Length

B. Friedman et al., Phys. Plasmas, 20:055704, 2013.



Brett Friedman, Troy Carter, Maxim Umansky, POSTER SESSION I

Principal Results since 2011 BOUT++ workshop



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  - ✓ **Coupled to EIRENE Monte Carlo code to follow the neutral particles.**
- **Developed Physics-based preconditioning based on Chacon's presentation at 2011 BOUT++ workshop**
- **We find that nonlinear mode coupling can shift the linear P-B mode stability threshold, which may explain those puzzles observed in ELM experiments.**

The mission of the 2013 BOUT++ Workshop

- **To provide a forum for the discussion of key physics and computational issues as well as innovative concepts of direct relevance to fluid, gyro-fluid plasma, and hybrid kinetic-fluid simulations**
- **To prepare researchers to use and further develop the BOUT++ code for simulations of turbulence, transport and ELMs in magnetic fusion devices**
- **To promote effective collaboration within the BOUT community and beyond**